

APPENDIX C

FLAMMABLE SUBSTANCES

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C.1 Equation for Estimation of Distance to 1 psi Overpressure for Vapor Cloud Explosions

For a worst-case release of flammable gases and volatile flammable liquids, the release rate is not considered. The total quantity of the flammable substance is assumed to form a vapor cloud. The entire contents of the cloud is assumed to be within the flammability limits, and the cloud is assumed to explode. For the worst-case analysis, 10 percent of the flammable vapor in the cloud is assumed to participate in the explosion (i.e., the yield factor is 0.10). Consequence distances to an overpressure level of 1 pound per square inch (psi) may be determined using the following equation, which is based on the TNT-equivalency method:

$$D = 17 \times \left(0.1 \times W_f \times \frac{HC_f}{HC_{TNT}} \right)^{1/3} \quad (\text{C-1})$$

where:	D	=	Distance to overpressure of 1 psi (meters)
	W _f	=	Weight of flammable substance (kilograms or pounds/2.2)
	H _{C_f}	=	Heat of combustion of flammable substance (kilojoules per kilogram) (listed in Exhibit C-1)
	H _{C_{TNT}}	=	Heat of explosion of trinitrotoluene (TNT) (4,680 kilojoules per kilogram)

The factor 17 is a constant for damages associated with 1.0 psi overpressures. The factor 0.1 represents an explosion efficiency of 10 percent. To convert distances from meters to miles, multiply by 0.00062.

Alternatively, use the following equation for quantity in pounds and distance in miles:

$$D_{mi} = 0.0081 \times \left(0.1 \times W_{lb} \times \frac{HC_f}{HC_{TNT}} \right)^{1/3} \quad (\text{C-2})$$

where:	D _{mi}	=	Distance to overpressure of 1 psi (miles)
	W _{lb}	=	Weight of flammable substance (pounds)

These equations were used to derive Reference Table 13 for worst-case distances to the overpressure endpoint (1 psi) for vapor cloud explosions.

C.2 Mixtures of Flammable Substances

For a mixture of flammable substances, you may estimate the heat of combustion of the mixture from the heats of combustion of the components of the mixture using the equation below and then use the equation given in the previous section of this appendix to determine the vapor cloud explosion distance. The heat of combustion of the mixture may be estimated as follows:

$$HC_m = \frac{W_x}{W_m} \times HC_x + \frac{W_y}{W_m} \times HC_y \quad (C-3)$$

where:

HC_m	=	Heat of combustion of mixture (kilojoules per kilogram)
W_x	=	Weight of component "X" in mixture (kilograms or pounds/2.2)
W_m	=	Total weight of mixture (kilograms or pounds/2.2)
HC_x	=	Heat of combustion of component "X" (kilojoules per kilogram)
W_y	=	Weight of component "Y" in mixture (kilograms or pounds/2.2)
HC_y	=	Heat of combustion of component "Y" (kilojoules per kilogram)

Heats of combustion for regulated flammable substances are listed in Exhibit C-1 in the next section (Section C.3) of this appendix.

C.3 Data for Flammable Substances

The exhibits in this section of Appendix C provide the data needed to carry out the calculations for regulated flammable substances using the methods presented in the text of this guidance. Exhibit C-1 presents heat of combustion data for all regulated flammable substances, Exhibit C-2 presents additional data for flammable gases, and Exhibit C-3 presents additional data for flammable liquids. The heats of combustion in Exhibit C-1 and the data used to develop the factors in Exhibits C-2 and C-3 are primarily from Design Institute for Physical Property Data, American Institute of Chemical Engineers, *Physical and Thermodynamic Properties of Pure Chemicals, Data Compilation*. The derivation of the factors presented in Exhibits C-2 and C-3 is discussed in Appendix D.

Exhibit C-1
Heats of Combustion for Flammable Substances

CAS No.	Chemical Name	Physical State at 25° C	Heat of Combustion (kjoule/kg)
75-07-0	Acetaldehyde	Gas	25,072
74-86-2	Acetylene [Ethyne]	Gas	48,222
598-73-2	Bromotrifluoroethylene [Ethene, bromotrifluoro-]	Gas	1,967
106-99-0	1,3-Butadiene	Gas	44,548
106-97-8	Butane	Gas	45,719
25167-67-3	Butene	Gas	45,200*
590-18-1	2-Butene-cis	Gas	45,171
624-64-6	2-Butene-trans [2-Butene, (E)]	Gas	45,069
106-98-9	1-Butene	Gas	45,292
107-01-7	2-Butene	Gas	45,100*
463-58-1	Carbon oxysulfide [Carbon oxide sulfide (COS)]	Gas	9,126
7791-21-1	Chlorine monoxide [Chlorine oxide]	Gas	1,011*
590-21-6	1-Chloropropylene [1-Propene, 1-chloro-]	Liquid	23,000*
557-98-2	2-Chloropropylene [1-Propene, 2-chloro-]	Gas	22,999
460-19-5	Cyanogen [Ethanedinitrile]	Gas	21,064
75-19-4	Cyclopropane	Gas	46,560
4109-96-0	Dichlorosilane [Silane, dichloro-]	Gas	8,225
75-37-6	Difluoroethane [Ethane, 1,1-difluoro-]	Gas	11,484
124-40-3	Dimethylamine [Methanamine, N-methyl-]	Gas	35,813
463-82-1	2,2-Dimethylpropane [Propane, 2,2-dimethyl-]	Gas	45,051
74-84-0	Ethane	Gas	47,509
107-00-6	Ethyl acetylene [1-Butyne]	Gas	45,565
75-04-7	Ethylamine [Ethanamine]	Gas	35,210
75-00-3	Ethyl chloride [Ethane, chloro-]	Gas	19,917
74-85-1	Ethylene [Ethene]	Gas	47,145

Exhibit C-1 (continued)

CAS No.	Chemical Name	Physical State at 25° C	Heat of Combustion (kjoule/kg)
60-29-7	Ethyl ether [Ethane, 1,1'-oxybis-]	Liquid	33,775
75-08-1	Ethyl mercaptan [Ethanethiol]	Liquid	27,948
109-95-5	Ethyl nitrite [Nitrous acid, ethyl ester]	Gas	18,000
1333-74-0	Hydrogen	Gas	119,950
75-28-5	Isobutane [Propane, 2-methyl]	Gas	45,576
78-78-4	Isopentane [Butane, 2-methyl-]	Liquid	44,911
78-79-5	Isoprene [1,3-Butadiene, 2-methyl-]	Liquid	43,809
75-31-0	Isopropylamine [2-Propanamine]	Liquid	36,484
75-29-6	Isopropyl chloride [Propane, 2-chloro-]	Liquid	23,720
74-82-8	Methane	Gas	50,029
74-89-5	Methylamine [Methanamine]	Gas	31,396
563-45-1	3-Methyl-1-butene	Gas	44,559
563-46-2	2-Methyl-1-butene	Liquid	44,414
115-10-6	Methyl ether [Methane, oxybis-]	Gas	28,835
107-31-3	Methyl formate [Formic acid, methyl ester]	Liquid	15,335
115-11-7	2-Methylpropene [1-Propene, 2-methyl-]	Gas	44,985
504-60-9	1,3-Pentadiene	Liquid	43,834
109-66-0	Pentane	Liquid	44,697
109-67-1	1-Pentene	Liquid	44,625
646-04-8	2-Pentene, (E)-	Liquid	44,458
627-20-3	2-Pentene, (Z)-	Liquid	44,520
463-49-0	Propadiene [1,2-Propadiene]	Gas	46,332
74-98-6	Propane	Gas	46,333
115-07-1	Propylene [1-Propene]	Gas	45,762
74-99-7	Propyne [1-Propyne]	Gas	46,165
7803-62-5	Silane	Gas	44,307

Exhibit C-1 (continued)

CAS No.	Chemical Name	Physical State at 25° C	Heat of Combustion (kjoule/kg)
116-14-3	Tetrafluoroethylene [Ethene, tetrafluoro-]	Gas	1,284
75-76-3	Tetramethylsilane [Silane, tetramethyl-]	Liquid	41,712
10025-78-2	Trichlorosilane [Silane, trichloro-]	Liquid	3,754
79-38-9	Trifluorochloroethylene [Ethene, chlorotrifluoro-]	Gas	1,837
75-50-3	Trimethylamine [Methanamine, N,N-dimethyl-]	Gas	37,978
689-97-4	Vinyl acetylene [1-Buten-3-yne]	Gas	45,357
75-01-4	Vinyl chloride [Ethene, chloro-]	Gas	18,848
109-92-2	Vinyl ethyl ether [Ethene, ethoxy-]	Liquid	32,909
75-02-5	Vinyl fluoride [Ethene, fluoro-]	Gas	2,195
75-35-4	Vinylidene chloride [Ethene, 1,1-dichloro-]	Liquid	10,354
75-38-7	Vinylidene fluoride [Ethene, 1,1-difluoro-]	Gas	10,807
107-25-5	Vinyl methyl ether [Ethene, methoxy-]	Gas	30,549

* Estimated heat of combustion

Exhibit C-2
Data for Flammable Gases

CAS Number	Chemical Name	Molecular Weight	Ratio of Specific Heats	Flammability Limits (Vol %)		LFL (mg/L)	Gas Factor (GF) ^g	Liquid Factor Boiling (LFB)	Density Factor (Boiling) (DF)	Reference Table ^a	Pool Fire Factor (PFF)	Flash Fraction Factor (FFF) ^f
				Lower (LFL)	Upper UFL							
75-07-0	Acetaldehyde	44.05	1.18	4.0	60.0	72	22	0.11	0.62	Dense	2.7	0.018
74-86-2	Acetylene	26.04	1.23	2.5	80.0	27	17	0.12	0.78	Buoyant ^b	4.8	0.23 ^f
598-73-2	Bromotrifluoroethylene	160.92	1.11	c	37.0	c	41 ^c	0.25 ^c	0.29 ^c	Dense	0.42 ^c	0.15 ^c
106-99-0	1,3-Butadiene	54.09	1.12	2.0	11.5	44	24	0.14	0.75	Dense	5.5	0.15
106-97-8	Butane	58.12	1.09	1.5	9.0	36	25	0.14	0.81	Dense	5.9	0.15
25167-67-3	Butene	56.11	1.10	1.7	9.5	39	24	0.14	0.77	Dense	5.6	0.14
590-18-1	2-Butene-cis	56.11	1.12	1.6	9.7	37	24	0.14	0.76	Dense	5.6	0.11
624-64-6	2-Butene-trans	56.11	1.11	1.8	9.7	41	24	0.14	0.77	Dense	5.6	0.12
106-98-9	1-Butene	56.11	1.11	1.6	9.3	37	24	0.14	0.78	Dense	5.7	0.17
107-01-7	2-Butene	56.11	1.10	1.7	9.7	39	24	0.14	0.77	Dense	5.6	0.12
463-58-1	Carbon oxysulfide	60.08	1.25	12.0	29.0	290	26	0.18	0.41	Dense	1.3	0.29
7791-21-1	Chlorine monoxide	86.91	1.21	23.5	NA	830	31	0.19	NA	Dense	0.15	NA
557-98-2	2-Chloropropylene	76.53	1.12	4.5	16.0	140	29	0.16	0.54	Dense	3.3	0.011
460-19-5	Cyanogen	52.04	1.17	6.0	32.0	130	24	0.15	0.51	Dense	2.5	0.40
75-19-4	Cyclopropane	42.08	1.18	2.4	10.4	41	22	0.13	0.72	Dense	5.4	0.23
4109-96-0	Dichlorosilane	101.01	1.16	4.0	96.0	160	33	0.20	0.40	Dense	1.3	0.084
75-37-6	Difluoroethane	66.05	1.14	3.7	18.0	100	27	0.17	0.48	Dense	1.6	0.23
124-40-3	Dimethylamine	45.08	1.14	2.8	14.4	52	22	0.12	0.73	Dense	3.7	0.090
463-82-1	2,2-Dimethylpropane	72.15	1.07	1.4	7.5	41	27	0.16	0.80	Dense	6.4	0.11
74-84-0	Ethane	30.07	1.19	2.9	13.0	36	18	0.14	0.89	Dense	5.4	0.75
107-00-6	Ethyl acetylene	54.09	1.11	2.0	32.9	44	24	0.13	0.73	Dense	5.4	0.091
75-04-7	Ethylamine	45.08	1.13	3.5	14.0	64	22	0.12	0.71	Dense	3.6	0.040

Exhibit C-2 (continued)

CAS Number	Chemical Name	Molecular Weight	Ratio of Specific Heats	Flammability Limits (Vol %)		LFL (mg/L)	Gas Factor (GF) ^g	Liquid Factor Boiling (LFB)	Density Factor (Boiling) (DF)	Reference Table ^a	Pool Fire Factor (PFF)	Flash Fraction Factor (FFF) ^f
				Lower (LFL)	Upper UFL							
75-00-3	Ethyl chloride	64.51	1.15	3.8	15.4	100	27	0.15	0.53	Dense	2.6	0.053
74-85-1	Ethylene	28.05	1.24	2.7	36.0	31	18	0.14	0.85	Buoyant ^b	5.4	0.63 ^f
109-95-5	Ethyl nitrite	75.07	1.30	4.0	50.0	120	30	0.16	0.54	Dense	2.0	NA
1333-74-0	Hydrogen	2.02	1.41	4.0	75.0	3.3	5.0	e	e	d	e	NA
75-28-5	Isobutane	58.12	1.09	1.8	8.4	43	25	0.15	0.82	Dense	6.0	0.23
74-82-8	Methane	16.04	1.30	5.0	15.0	33	14	0.15	1.1	Buoyant	5.6	0.87 ^f
74-89-5	Methylamine	31.06	1.19	4.9	20.7	62	19	0.10	0.70	Dense	2.7	0.12
563-45-1	3-Methyl-1-butene	70.13	1.08	1.5	9.1	43	26	0.15	0.77	Dense	6.0	0.030
115-10-6	Methyl ether	46.07	1.15	3.3	27.3	64	22	0.14	0.66	Dense	3.4	0.22
115-11-7	2-Methylpropene	56.11	1.10	1.8	8.8	41	24	0.14	0.77	Dense	5.7	0.18
463-49-0	Propadiene	40.07	1.16	2.1	2.1	34	21	0.13	0.73	Dense	5.2	0.20
74-98-6	Propane	44.10	1.13	2.0	9.5	36	22	0.14	0.83	Dense	5.7	0.38
115-07-1	Propylene	42.08	1.15	2.0	11.0	34	21	0.14	0.79	Dense	5.5	0.35
74-99-7	Propyne	40.07	1.16	1.7	39.9	28	21	0.12	0.72	Dense	4.9	0.18
7803-62-5	Silane	32.12	1.24	c	c	c	19 ^c	e	e	Dense	e	0.41 ^f
116-14-3	Tetrafluoroethylene	100.02	1.12	11.0	60.0	450	33	0.29	0.32	Dense	0.25	0.69
79-38-9	Trifluorochloroethylene	116.47	1.11	8.4	38.7	400	35	0.26	0.33	Dense	0.34	0.27
75-50-3	Trimethylamine	59.11	1.10	2.0	11.6	48	25	0.14	0.74	Dense	4.8	0.12
689-97-4	Vinyl acetylene	52.08	1.13	2.2	31.7	47	24	0.13	0.69	Dense	5.4	0.086
75-01-4	Vinyl chloride	62.50	1.18	3.6	33.0	92	26	0.16	0.50	Dense	2.4	0.14
75-02-5	Vinyl fluoride	46.04	1.20	2.6	21.7	49	23	0.17	0.57	Dense	0.28	0.37
75-38-7	Vinylidene fluoride	64.04	1.16	5.5	21.3	140	27	0.22	0.42	Dense	1.8	0.50

Exhibit C-2 (continued)

CAS Number	Chemical Name	Molecular Weight	Ratio of Specific Heats	Flammability Limits (Vol %)		LFL (mg/L)	Gas Factor (GF) ^g	Liquid Factor Boiling (LFB)	Density Factor (Boiling) (DF)	Reference Table ^a	Pool Fire Factor (PFF)	Flash Fraction Factor (FFF) ^f
				Lower (LFL)	Upper UFL							
107-25-5	Vinyl methyl ether	58.08	1.12	2.6	39.0	62	25	0.17	0.57	Dense	3.7	0.093

Notes:

NA: Data not available

^a "Buoyant" in the Reference Table column refers to the tables for neutrally buoyant gases and vapors; "Dense" refers to the tables for dense gases and vapors. See Appendix D, Section D.4.4, for more information on the choice of reference tables.

^b Gases that are lighter than air may behave as dense gases upon release if liquefied under pressure or cold; consider the conditions of release when choosing the appropriate table.

^c Reported to be spontaneously combustible.

^d Much lighter than air; table of distances for neutrally buoyant gases not appropriate.

^e Pool formation unlikely.

^f Calculated at 298 K (25 °C) with the following exceptions:

Acetylene factor at 250 K as reported in TNO, *Methods for the Calculation of the Physical Effects of the Escape of Dangerous Material* (1980).

Ethylene factor calculated at critical temperature, 282 K.

Methane factor calculated at critical temperature, 191 K.

Silane factor calculated at critical temperature, 270 K.

^g Use GF for gas leaks under choked (maximum) flow conditions.

Exhibit C-3
Data for Flammable Liquids

CAS Number	Chemical Name	Molecular Weight	Flammability Limit (Vol%)		LFL (mg/L)	Liquid Factors		Density Factor	Liquid Leak Factor (LLF) ^a	Reference Table ^b	Pool Fire Factor (PFF)
			Lower (LFL)	Upper (UFL)		Ambient (LFA)	Boiling (LFB)				
590-21-6	1-Chloropropylene	76.53	4.5	16.0	140	0.11	0.15	0.52	45	Dense	3.2
60-29-7	Ethyl ether	74.12	1.9	48.0	57	0.11	0.15	0.69	34	Dense	4.3
75-08-1	Ethyl mercaptan	62.14	2.8	18.0	71	0.10	0.13	0.58	40	Dense	3.3
78-78-4	Isopentane	72.15	1.4	7.6	41	0.14	0.15	0.79	30	Dense	6.1
78-79-5	Isoprene	68.12	2.0	9.0	56	0.11	0.14	0.72	32	Dense	5.5
75-31-0	Isopropylamine	59.11	2.0	10.4	48	0.10	0.13	0.71	33	Dense	4.1
75-29-6	Isopropyl chloride	78.54	2.8	10.7	90	0.11	0.16	0.57	41	Dense	3.1
563-46-2	2-Methyl-1-butene	70.13	1.4	9.6	40	0.12	0.15	0.75	31	Dense	5.8
107-31-3	Methyl formate	60.05	5.9	20.0	140	0.10	0.13	0.50	46	Dense	1.8
504-60-9	1,3-Pentadiene	68.12	1.6	13.1	44	0.077	0.14	0.72	33	Dense	5.3
109-66-0	Pentane	72.15	1.3	8.0	38	0.10	0.15	0.78	30	Dense	5.8
109-67-1	1-Pentene	70.13	1.5	8.7	43	0.13	0.15	0.77	31	Dense	5.8
646-04-8	2-Pentene, (E)-	70.13	1.4	10.6	40	0.10	0.15	0.76	31	Dense	5.6
627-20-3	2-Pentene, (Z)-	70.13	1.4	10.6	40	0.10	0.15	0.75	31	Dense	5.6
75-76-3	Tetramethylsilane	88.23	1.5	NA	54	0.17	0.17	0.59	40	Dense	6.3
10025-78-2	Trichlorosilane	135.45	1.2	90.5	66	0.18	0.23	0.37	64	Dense	0.68
109-92-2	Vinyl ethyl ether	72.11	1.7	28.0	50	0.10	0.15	0.65	36	Dense	4.2
75-35-4	Vinylidene chloride	96.94	7.3	NA	290	0.15	0.18	0.44	54	Dense	1.6

Notes:

NA: Data not available.

^a Use the LLF only for leaks from tanks at atmospheric pressure.

^b "Dense" in the Reference Table column refers to the tables for dense gases and vapors. See Appendix D, Section D.4.4, for more information on the choice of reference tables.